CHAPTER 8

Searching For Polymers

DONNA T. WRUBLEWSKI

California Institute of Technology, 1200 E. California Blvd., MC 1-43, Pasadena, CA 91125, US
Email: dtwrublewski@library.caltech.edu

8.1 INTRODUCTION

A polymer is broadly defined as a substance made up of many linked atoms or smaller molecules. Unlike small molecules, polymer properties can vary considerably depending on the method of synthesis, measurement technique, and experimental conditions. As such, knowing additional information about the polymer of interest can be helpful when searching for specific information. This chapter outlines some of this additional information to aid in searching primary literature, and also includes references to secondary compendia where possible.

Section 8.2 covers polymer structure nomenclature and searching; although progress is being made towards a more uniform naming system, as with other areas of chemistry, there are colloquial as well as systematic names in use currently and particularly in older literature. Section 8.3 briefly describes common methods of polymer synthesis, as different synthetic methods applied to the same monomer can produce polymers with significantly different properties. Methods for characterization of polymer structure are discussed in Section 8.4, as different methods may yield different values for a property. Sections 8.5 and 8.6 describe some of the most common thermophysical and

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mechanical properties of interest, respectively. Concluding remarks are offered in Section 8.7, along with a general bibliography for further background information.

8.2 POLYMER NOMENCLATURE AND STRUCTURE

In addition to standard text searching, chemical literature can also be searched *via* chemical structure. Basic text name searching will be discussed in Section 8.2.1 and structure-based searching is covered in Section 8.2.2.

8.2.1 Text Name Searching

There are three types of nomenclature currently in use for polymers: formal methodic scientific nomenclature systems, common colloquial names rooted in history, and commercial trade names. A thorough search should include as many names as possible, particularly when dealing with historic literature.

Historically, two classes of nomenclature systems have existed for the naming of polymers: source-based and structure-based. Overviews of each system can be found in several reference books, including the *Polymer Handbook*[1] and the most recent *CRC Handbook*,[2] as well as in introductory-level polymer chemistry texts such as that by Odian.[3] Source-based naming derives the polymer name from the monomer or monomers that form the polymer. Structure-based names are determined by examining the final structure of the polymer and identifying a repeating subunit. The International Union of Pure and Applied Chemistry recently published a compendium describing guidelines for a broad range of polymer terminology including nomenclature,[4] and recommend a structure-based nomenclature system for linear homopolymers that names polymers according to the smallest repeating subunit. However, for very common commercial polymers, this system is not expected to supplant established names. One example of this is polyethylene, so named for its formation from the monomer ethylene. The most basic structural repeat unit is that of the methylene group ($-CH_2-$), so IUPAC rules dictate the name should be polymethylene. Searching for polymethylene will yield very different results than for polyethylene; the former should be included to ensure older historical literature is retrieved. It is recommended to search for the IUPAC name in conjunction with the common name, should one exist.

Common established polymer names are frequently made up of several words, and the same name can often be written in more than one

way. An example of this would be the terms *poly(ethylene oxide)* versus *polyethylene oxide*. In general discussion, parentheses should be used to write the polymer name when the monomer name contains multiple words or contains substituent position numbers.[5] However, when searching, it is important to know the specific database parameter, particularly if it is one with broad or non-specific subject coverage. For example, Thompson Reuters' Web of Knowledge platform executes Boolean expressions inside parentheses first.[6] For a Topic search with this example, parentheses are ignored and in the absence of a Boolean operator, *poly(ethylene oxide)* is searched as *poly* AND *ethylene* AND *oxide* and retrieves over 18,000 records. Similarly, *polyethylene oxide* is searched as *polyethylene* AND *oxide*, retrieving over 7,500 records. The first set will obviously include irrelevant records, while the second will likely be missing some relevant articles. Possible strategies for optimizing search results would include:

(1) Searching for "polyethylene oxide" OR "poly ethylene oxide" as phrases, which retrieves over 16,800 records from a Web of Knowledge Topic search, or, alternatively, over 5,300 from a Title search.
(2) Including additional terms, such as abbreviations or trade names, or other polymer-specific properties, thereby possibly eliminating references to small molecules.

Two general sources for polymer trade names and abbreviations are Section VIII in the *Polymer Handbook* (fourth edition)[7] and Appendix II in *Contemporary Polymer Chemistry*.[8] The *Polymer Data Handbook* is organized by polymer type, and lists trade names and abbreviations for many classes of polymers. The CAS Registry by default includes abbreviations and trade names in its comprehensive listings, and will be discussed later in this section.

Another type of compound name is encountered when dealing with copolymers. Source-based names can include multiple monomers, as well as the designation of the type of copolymer. The most common descriptors seen with copolymers are –co– (unspecified or unknown structure), –block– (monomers are in defined blocks within the polymer), and –alt– (monomer units alternate within the polymer), although others are becoming more common, along with more formal IUPAC designations for structures.[2] When searching for copolymers, it is helpful to not only search a polymer name (such as *poly(styrene-co-butadiene)*) but also phraseology such as "styrene butadiene copolymer" or "block copolymer" (if the type of copolymer structure is known). Trade names and abbreviations are also very common in the copolymer

field, and can significantly enhance the relevance of searches if they are known.[7,8]

Terms relating to polymer stereochemistry can often be helpful in searching for information. Tacticity generally refers to the orientation of substituents on a (usually saturated) polymer backbone chain relative to the plane of the chain itself.[9] Substituents with periodic repetition located on the same side of the plane are referred to as isotactic, whereas if they are on opposite sides of the plane they are called syndiotactic. If a chain has no order to the placement of substituents relative to the plane, it is referred to as atactic. Usually these terms (or their abbreviations i-, s-, and a-) are used in conjunction with the polymer name, and can be used to narrow down a search if known. For unsaturated backbones, such as polyisoprene, another type of tacticity can also exist, that of transtactic and cistactic. For planar double bonds, *cis* refers to the polymer chain bonds being on the same side of the double bond, and *trans* if they are on opposite sides. Tacticity can have a significant effect on polymer properties, such as glass transition temperature and crystallinity, and thus should be included, if relevant, in searching for specific properties (*i.e., "isotactic polypropylene"*).

8.2.2 Structure Searching

Small molecules, including monomers and some oligomers, can be searched by chemical structure in some databases, including the CAS Registry (accessible through the SciFinder or STN platforms).[10] Elsevier's Reaxys, NCBI's PubChem, and RSC's ChemSpider. Structures can be entered using text representation systems, such as the IUPAC International Chemical Identifier (InChI) or the Simplified Molecular-Input Line-Entry System (SMILES). Alternatively, on some platforms, structures can be drawn directly using embedded structure editors. Currently, there is no formal standard for polymer representation using SMILES notation,[11] however, development is ongoing in that area.[12] Also, development for InChI representation of polymers is ongoing but not standardized or widely adopted.[13] As such, there is limited support for polymer searching by full structure in any major database, but several do support searching by monomer structure. Examples of how to do this using Elsevier's Reaxys and the CAS Registry are in the following sections.

8.2.2.1 Reaxys. At the time of this writing, Reaxys has very limited retrieval of polymers using the "Structure and Properties" search facet, since it does not index polymers by structure. This includes patented and trade materials, as well as broad polymer groups. Some

common polymers, such as polyethylene, can be searched using the "Generate structure from name" feature, however this will result in only the repeating unit (-CH2-CH2-) being identified and searched. More relevant, but again limited, results can be found by searching under the "Substances and Properties" function, selecting "Properties (Advanced)", then "Identification", then "Substance Identification", and populating the "Chemical Name" form with the prefix *poly* to generate a list of polymer names.

Another approach would be to use the "Reactions" function, and drawing or generating a monomer (or monomers) of interest and selecting "Starting material" under "Search as by". Under "Conditions (Form-based)", the "Product name" form can be populated using the "starts with" option and the prefix *poly* to generate a list of index terms of possible polymer products. Of note here is that the Beilstein database, on which Reaxys is based, historically never indexed polymers, although the Gmelin database (also included in Reaxys) did include a limited number of inorganic polymers. It does appear though that, as with other sources, coverage is increasing due to indexing from journal articles and patents.

8.2.2.2 The CAS Registry Database. The CAS Registry is a specialized chemical substance database that, as of this writing, contains substance information, including names, structure, and property data, for over 70 million compounds, mostly small molecules and oligomers, each with a uniquely assigned CAS Registry Number (CAS RN).[10] An overview of the CAS Registry organization, as well as a list of CAS RN's for some common polymers, can be found in Section VIII of the *Polymer Handbook*.[14] Since the time of that publication, the coverage of the CAS Registry has grown exponentially and has become available on the SciFinder platform in addition to STN platform. Both platforms allow for structure searching by text or by drawing, but again are primarily limited to monomer structures. One advantage, however, of using a CAS RN to search is that unique chemical moieties have unique CAS RNs: chemicals with the same structure but different types of isomerism would have different CAS RNs, which can be helpful when searching for polymers with specific tacticity or activity. Knowing the CAS RN can also be of use when searching other resources that index them, including databases such as PubChem as well as vendor catalogs.

The SciFinder "Explore Substances" search facet allows searching of the CAS Registry by several fields. The three that will be discussed here in relation to polymers are "Substance Identifier", "Chemical Structure", and "Molecular Formula". The result of any search for a

polymer will be a list of substances organized by CAS RN, and will include known alternate names (which can be helpful for text name searching), the molecular structure and CAS RN of any component monomers, and molecular property and spectral information for the polymer, if available, with references.

For common polymers, searching by name in the "Substance Identifier" field will usually identify the polymer. As in Reaxys, polymers with specific components (including many patented and trade materials, and broad groups such as polycarbonates) usually will not have structure information available. When using the "Chemical Structure" search facet, the structure of the monomer(s) of interest can be drawn, and the search can be limited to the "Polymers" Class. Polymers which cannot be found via a substance identifier search might be located if the component monomer(s) can be drawn and searched. The "Molecular Formula" field search allows searching by repeat unit, grouped by parentheses, followed by "x"; an example is *(C2H4)x* for polyethylene. For copolymer searches, include the formulae for each monomer separated by a period, such as *(C2H4.C2H4O)x* for co-polymers of ethene and ethylene oxide.

8.3 POLYMER SYNTHESIS

When searching for polymerization reactions, either in general or with respect to a specific polymer as a product, it is helpful to know the reactants, mechanism, and reaction conditions, as with any chemical reaction. Including the polymerization mechanism (chain growth or step growth; cationic or anionic; ring opening metathesis polymerization, also known as ROMP; *etc.*) in a search for a specific polymer and product characteristics such as target molar mass or tacticity can increase the relevance of search results. Overviews of common types of polymerization reactions can be found in many introductory-level polymer science texts. The synthesis of both general polymer types as well as industrially important materials can be found in the first two volumes of the work of Elias[15] as well as other references listed at the end of this chapter. When searching for polymers, particularly those that may be synthesized by more than one mechanism, including the polymer name and the desired polymerization method or reaction in a Boolean search strategy is recommended (*i.e.*, polystyrene, which can be made by either cationic or anionic mechanisms).

One common polymerization reaction parameter often desired is the rate constant. This value will depend heavily on the monomer(s), the type of polymerization, and the reaction conditions. A comprehensive

list of reaction rates and reactivity ratios can be found in Section II of the *Polymer Handbook*.[16]

8.4 POLYMER STRUCTURE CHARACTERIZATION

As mentioned earlier, unlike small molecules, polymer molecules can have a range of properties, based not only on structure but also on differing molar masses with the same basic structure. This section will discuss the basics of molar mass properties and polymer structures, as well as characterization methods by which they are determined, since different methods can yield different results. As with synthesis information, it can be helpful to include the specific measurement technique when searching for a polymer so that the values obtained can be interpreted in context. Section 8.4.1 will discuss techniques and terminology related to molar mass measurements. Section 8.4.2 will briefly describe spectroscopic techniques frequently employed to determine polymer chemical structure. Physical structure characterization is treated in Section 8.4.3.

8.4.1 Molar Mass and Dispersity

In keeping with recent texts,[4,17] the terms "molar mass" and "dispersity" will be used here instead of molecular weight and polydispersity index, although the latter are still in common usage and prevalent in older literature. Molar mass is the weight of one mole of polymer molecules. Molecular weight is more correctly defined as the dimensionless relative molecular mass. The most common types of molar mass measured are the number-average (M_n), weight-average (M_w), and z-average (M_z). The dispersity of a polymer system is defined as the ratio of the weight-average molar mass to the number-average molar mass.

Different measurement techniques may yield different values for these properties. Techniques based on size exclusion chromatography (SEC), such as gel permeation chromatography (GPC), can determine the entire molar mass distribution of a polymer but require comparison with a well-characterized standard material.[18] Static light scattering (sometimes abbreviated as SLS) can be an effective way to determine an absolute value for M_w, as well as other molecular properties, and dynamic light scattering (DLS) can be used to determine properties such as diffusion coefficient and hydrodynamic radius.[19] Mass spectroscopy is another method of characterizing structure and molar mass, but until recently was only applicable to low molar mass compounds.[20]

Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) is a method applying this technique to high molecular weight compounds, and is based on polymer chains associating with ions in the vapor phase. Measuring the time of flight of the polymer ion complex through an applied electromagnetic field will give a distribution of travel times, with heavier species taking longer to travel through the detector.[21]

Because of the relationship between measured properties and molar mass, it is important to have a general idea of the molar mass range of interest when searching for property data. Likewise, when evaluating property data, it is important to be aware of the molar mass range and measurement technique for which it has been measured. When searching the primary literature with Boolean operators, molar mass ranges and measurement techniques (full names and acronyms) should be included in the search string construction, keeping in mind the terms used in older literature discussed previously. Of the secondary sources available, the *Polymer Data Handbook*[22] specifically compiles molar masses by trade name within polymer classes and types. For light scattering, a listing of scattering factors can be found in Section VII of the *Polymer Handbook*.[14]

8.4.2 Spectral Analyses

Many types of spectral analyses are useful for elucidating polymer structure. Brief descriptions will be given here for infrared spectroscopy, Raman spectroscopy, and nuclear magnetic resonance spectroscopy, along with pertinent search terms and recommended sources.

Infrared (IR) and Raman spectroscopy are both based on the interaction of infrared radiation with chemical bonds. IR spectroscopy measures the absorption of specific frequencies in the IR spectrum by chemical bonds that produce a change in dipole moment under irradiation.[23] IR spectra are used primarily for identification of substances by measuring the characteristic frequencies associated with specific molecular motions. Many current machines, usually of the Fourier Transform (FT-IR) type, come with software containing a database of established spectra and will automatically identify samples analyzed. Another type of IR is attenuated total reflectance (ATR-IR), which allows for surface characterization.

Raman spectroscopy is based on measuring the frequency change of inelastically scattered light.[24] Like IR, Raman is used to measure specific chemical bond energy properties, but it can also detect morphological changes as well. Less specific sample preparation is needed than with IR, so it can be employed in more environments, such as in-situ monitoring of polymerization reactions.

Nuclear magnetic resonance (NMR) spectroscopy is based on the principle of magnetic spin and measures radiation absorption (in the range of 1–500MHz) relative to a reference compound.[25] NMR spectroscopy usually measures ^{1}H or ^{13}C absorptions of polymers in solution, and can be used to determine more detailed microstructural information, such as tacticity, than that obtained *via* IR or Raman. Many types of advanced analysis techniques exist for NMR, including two-dimensional correlation spectroscopy (2D COSY) among others. Including these types of analysis techniques can be helpful in searching for information.

One of the most extensive collections of Raman, IR, NMR, and other spectra is the Sadtler Standard Spectra collection. Still available in many libraries in print, the collection was purchased from Sadtler Research Labs in 1978 by Bio-Rad, which currently maintains the electronic version of these spectral databases.[26,27] The print collection can be searched by indexes if information such as name, molecular formula, or chemical type is known. Recently, some spectra from the Bio-Rad electronic collection have been made available as part of substances' CAS Registry records, accessible via SciFinder and STN, and can be found by searching the CAS Registry for specific substances as discussed previously. While SciFinder does not generally index spectral data if it is used purely for characterization purposes, checking the full text of the original articles dealing with the synthesis of a compound may provide said data. Reaxys also allows searching by spectral availability and provides links to primary source data.

Some spectral data, such as NMR shifts and IR absorption frequencies, can be found for certain polymers in the *Polymer Data Handbook*[22] and in Section V of the *Polymer Handbook*.[16] Absorption tables for common chemical moieties exist in organic and polymer chemistry textbooks, such as that by Silverstein.[28] Tables of standard values for chemical shifts can be found in many textbooks and are often incorporated into equipment software and analysis. As before, when searching the primary literature it is helpful to include the specific type of technique or spectra desired (*i.e.*, ^{13}NMR as opposed to simply NMR).

8.4.3 X-Ray Diffraction and Scattering Analysis of Structure

X-ray Diffraction (XRD), Wide Angle X-ray Scattering (WAXS), and Small Angle X-ray Scattering (SAXS) are used to elucidate crystalline and semicrystalline phases in polymers that are capable of crystallization.[29] Technically, diffraction refers to the scattering pattern produced by the interaction of X-rays with regular features (such as crystals) in molecules. The size of a crystalline unit cell can be calculated from measuring the spacing of features in these patterns. Crystal

symmetry systems, both plane and space groups, are compiled by the International Union of Crystallography in the International Tables.[30]

Scattering techniques measure scattered radiation (X-ray) intensity as a function of scattering angle.[31] WAXS studies can measure the spacing between individual chains in ordered regions and from this the degree of crystallinity and density can be calculated. SAXS can yield information about slightly larger molecular structures, including crystal thickness and periodicity. Crystallinity can be highly system-dependent, so it is important when searching the primary literature to include conditions such as molar mass, density, tacticity, measurement technique, and composition, if known (particularly for copolymers).

Crystallographic data, including space group information and unit cell parameters, for some polymers can be found in Section V of the *Polymer Handbook*[16] and the *Polymer Data Handbook*.[22] The Cambridge Structural Database and WebCSD[32] also include crystallographic data for some polymers, but is only searchable through a "Text Numeric Search" and using "Compound Name", or entering the molecular formula in an "All Text" search. In SciFinder, when retrieving references from a "Substance Detail", it is possible to limit to those references containing "Crystal Structure" information.

8.5 POLYMER THERMOPHYSICAL PROPERTIES

This section describes a few of the most common thermophysical properties of polymers for which data is often desired. Many electronic resources, including SciFinder, Reaxys, and the *CRC Handbook of Chemistry and Physics*, have recently incorporated the ability to search by a specific value or range of values for a property of interest, instead of by substance. This includes some of the previously discussed properties such as spectra, and will include the properties discussed in Section 8.6. In general, searching by property value alone will yield relevant results provided the chosen database has an adequate amount of indexed property data and contains substances with the desired property value. If searching by property value fails to yield relevant information, searching primary literature by substance and property name is recommended.

8.5.1 Glass Transition, Melting, and Decomposition Temperatures

The types of thermophysical properties available for any given polymer will depend on its structure. Polymers can have the same chemical structure, but have significantly different physical structures depending on their formation conditions and processing conditions. One of the most important properties is the glass transition temperature (T_g). Most

small molecules do not possess this transition due to significant order in the solid state – therefore, usually only a melting temperature is reported. Furthermore, for highly regular structures, this temperature will not vary by measurement method. Amorphous polymers will usually only display a glass transition temperature. Semi-crystalline or crystalline polymers may exhibit T_g in addition to T_m.

As mentioned previously, XRD is one way to determine crystallinity of polymers. Differential Scanning Calorimetry (DSC) is another technique used to measure crystallinity as well as glass and melting transitions, and heat capacity. It is based on measuring heat flow into (or temperature change of) a sample compared to a reference material.[33] The main experimental parameter in DSC is the rate of change in the heating element, as this affects the measured transition temperatures, and should be noted when searching for values listed above measured with this technique.

Glass transition and melting values for common polymers can be found in most introductory texts, the *Polymer Data Handbook*.[22] Section V of the *Polymer Handbook*,[16] and Section 13 of the *CRC Handbook of Chemistry and Physics*.[34] Attention should be paid to the method by which the value was determined.

The decomposition temperature of a polymer may be needed for specific applications, or for determining other experimental parameters. Usually this is measured *via* thermogravimetric analysis (TGA), which measures mass loss as a function of temperature. TGA experiments can be carried out at different heating rates in a variety of gaseous environments such as air, pure oxygen, or pure nitrogen, with or without humidity. These conditions should be included, if known, when searching for decomposition information in the primary literature. A compilation of common polymer decomposition temperatures and corresponding decomposition products is given in Section II of the *Polymer Handbook*.[35]

8.5.2 Polymer Solubility and Miscibility

Polymer solubility has implications for many experimental applications, including synthesis and characterization. When designing an experiment that requires a polymer solution, a list of common solvents can be found in Section 13 of the *CRC Handbook of Chemistry and Physics*.[34] More data for solvents can also be found in Section III of the *Polymer Handbook*.[16] Potential solvents can be used in conjunction with the polymer of interest to search the primary literature. Where water is the solvent of interest, the *CRC Handbook of Thermodynamic Data of Aqueous Polymer Solutions* provides solubility and other

thermodynamic data for a number of polymers,[36] and the same is provided for copolymer solutions in a companion volume.[37]

Solubility is also directly related to polymer solution phase behavior, particularly in terms of upper critical solution temperatures (UCST) or lower critical solution temperatures (LCST). Again, some values are tabulated,[38] but including UCST or LCST terms in searches will help narrow down the desired phase properties.

8.6 POLYMER MECHANICAL AND ENGINEERING PROPERTIES

As noted for Section 8.5, several electronic databases allow for searching by property value. Again, should searching by property value provide inadequate information, searching the primary literature by substance and property name is recommended. Of particular note here is the common use of commercial materials for many polymer engineering studies, and a good source of property data for common commercially available materials is MatWeb,[39] where data is usually provided from commercial suppliers and MSDS sheets.

8.6.1 Viscoelastic Behavior

Due to the long chain molecular structure of polymers, their mechanical behavior is referred to as viscoelastic – a combination between that of a viscous fluid and an elastic solid. The mechanical properties of polymers are related by what is commonly called the *time temperature superposition (TTS) principle*.[40] In essence, this states that properties measured at a high rate are equivalent to properties measured at a low temperature, and *vice versa*. This is due to the effect of rate and temperature on molecular mobility. At low temperatures, there is less thermal energy to effect molecular rearrangement, and at high rates there is less time. At high temperatures, there is more thermal energy to effect molecular rearrangement, and at low rates there is more time. As such, when searching for particular property values, it is important to know beforehand the experimental conditions of interest, and to be aware of the conditions under which reported values are obtained. The first of the following two sections covers low-rate testing (usually referred to as static or quasi-static conditions), and the second covers high-rate testing (referred to as dynamic conditions).

8.6.2 Static Testing

Common static mechanical properties of relevance include tensile (or Young's) modulus, compressive modulus, shear modulus, ultimate

tensile strength, and Poisson's ratio. Occasionally the term *compliance* is seen instead of modulus, and is the reciprocal of the modulus. Temperature of measurement, particularly with respect to the glass transition temperature of the material, is vital, as properties can change drastically even over the course of a fraction of a degree if in proximity to T_g. Rate of testing is also important, although properties tend not to vary much as long as the rate can be considered static or quasi-static.

Several secondary sources already mentioned provide mechanical property data for many polymers. Section 13 of the *CRC Handbook of Chemistry and Physics* provides strength data for nineteen common industrial polymers.[34] Section V of the *Polymer Handbook*[16] as well as the *Polymer Data Handbook*[22] both provide mechanical property data for many polymers, but are more easily navigable by polymer name than by property value.

When searching primary literature, properties such as molecular weight, temperature, and rate of testing should be included along with polymer name or structure. However, these properties can vary significantly by molar mass and crystallinity, so these additional parameters should be included if known.

8.6.3 Dynamic Testing

Dynamic mechanical properties, such as storage modulus, loss modulus, tan delta (the ratio of loss modulus to storage modulus) and dynamic viscosity are specific to both temperature and frequency of measurement, as well as to the intrinsic polymer properties. They can also vary by instrumentation used; a Dynamic Mechanical Analyzer (DMA) may give different data than a rheometer. When searching for or evaluating dynamic data, the experimental conditions (such as temperature or shearing rate, and frequency or frequency spectrum) should be well noted. Dynamic data is reported for some polymers in the *Polymer Data Handbook*.[22]

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8.8 CONCLUSIONS

Searching for polymer information, like other types of chemical information, is challenged by both the changing nature of search interfaces and subject databases, as well as the evolution of the nomenclature and structure representation itself. An added complication is the dependence of polymer properties on both physical (in addition to chemical) structure as well as the method of measurement. Secondary sources and data compilations should be consulted whenever possible, but attention should be paid to the caveats above when reporting data. When searching the primary literature, knowing specific information of interest, such as substance properties or characterization techniques, can facilitate finding relevant information.

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